

Ising low-temperature polynomials and hard-sphere gases on cubic lattices of general dimension

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We derive and analyze the low-activity and low-density expansions of the pressure for the model of a hard-sphere gas on cubic lattices of general dimension d , through the 13th order. These calculations are based on our recent extension to dimension d of the low-temperature expansions for the specific free-energy of the spin-1/2 Ising models subject to a uniform magnetic field on the (hyper-)simple-cubic lattices. Estimates of the model parameters are given also for some other lattices.

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I. INTRODUCTION

A simpler and mathematically more tractable discretization of the long-studied hard-sphere fluid in continuum space is called “hard-sphere lattice gas” (HSLG) with nearest-neighbor exclusion^{1–5}. In this model the sites of a regular lattice are the only allowed positions of the constituents. The pair interaction potential is $+\infty$ for constituents centered on nearest-neighbor sites and vanishes otherwise. Double occupancy of sites is forbidden. In particular in $2d$, on a square (sq) lattice, the spheres of the model can be viewed as “hard-squares” oriented at $\pi/4$ with respect to the lattice axes and whose diagonals equal two lattice spacings. In $3d$ the spheres are effectively “hard octaedra” and analogously for higher-dimensional lattices, they are polytopes (i.e. convex hyper-polyhedra) whose vertices are the nearest neighbors of the sites on which they are centered.

If the properties of the HSLG on a finite lattice are described by the statistical mechanics formalism of the grand partition function, it turns out that the n th coefficient of the low-activity(LA) series-expansion of the grand-potential has the same combinatorial definition^{3–5} as the coefficient of the highest power of the temperature-like variable u in the n th low-temperature (LT) polynomial of a ferromagnetic Ising model with spin $S = 1/2$ on the same lattice. This relationship remains valid when the thermodynamic limit is taken. When this fact was recognized, it became trivial to write down the LA expansions of the pressure once the LT expansion of the Ising model on the same lattice, in presence of a magnetic field, is known.

Thus, for the one-dimensional lattice, one can write a LA expansion valid to all orders. For the sq lattice, initially the LA expansion could be obtained^{3–5} in this way only through the 12th order. The derivation was later extended⁶ through the 21st order. Finally, by a more powerful approach based on the corner-transfer-matrix method⁷, the LA series was pushed through the 42nd order and more recently⁸ through the 92nd order.

For the triangular lattice (“*hard-hexagon*” model), an exact solution^{9,10} of the HSLG model was devised. It is expected¹¹ that also the honeycomb (hc) lattice case (called the “*hard-triangle*” model) is soluble, however, presently we know only a 25th order LA expansion derived from the LT Ising expansion^{12,13} for the hc lattice. For lattices of dimension $d > 2$, the transfer-matrix techniques are not efficient, so that one has to rely only on the LT Ising expansions and no LA data of extension comparable with that of the sq lattice can be derived. In the case of the three-dimensional hydrogen-peroxide (hpo) lattice, a bipartite cubic lattice of coordination number 3, the known Ising LT series¹⁴ yields a 23rd order LA series for the HSLG model. For the three-dimensional bipartite *diamond* lattice, with coordination number 4, the first 17 LA coefficients can be obtained¹⁵. Only the first 15 Ising LT polynomials are presently known^{6,16} for the simple-cubic (sc) lattice in $3d$ and the hyper-simple-cubic (hsc) in $4d$, while the first 11 polynomials¹⁷ are known in the case of the body-centered-cubic (bcc) lattice. No LT data at all existed up to now for the hsc and the hyper-body-centered-cubic ($hbcc$) lattices of dimension $d > 4$.

We have recently calculated¹⁸ the Ising LT polynomials for all hsc lattices in general dimension d through the 13th order. As a result, in this paper we can present the LA and low-density (LD) expansions for the HSLG through the same order, having observed that the LD expansion coefficients $v_k(d)$ of the pressure are polynomials of degree $\lfloor \frac{k}{2} \rfloor$ in

d. It is worth noticing that also the LD expansion coefficients of the pressure for the dimer model on the *hsc* lattices share a similar (slow) polynomial dependence on d , making it possible to determine¹⁹ the LD expansions through the 20th order.

We shall analyze the LA expansions for the HSLG to extract information about the properties of the model for $d > 4$, which, up to now, have been the subject of a single accurate MonteCarlo(MC) study²⁰. To support some of the indications suggested from our study for the higher-dimensional lattices, we shall also perform an analysis of the LA and the LD series for the *hc*, the *hpo* and the *diamond* lattices, to which little attention was devoted in the literature.

It is also well known that, using the standard correspondence² between the lattice gas and the spin-1/2 Ising model, one can relate the HSLG with an LT anti-ferromagnetic Ising spin system subject to a magnetic field^{3,21,22} on the same lattice and thus further insight can come also from this standpoint. In particular, in analogy with the LA series, the high-activity (HA) expansions coefficients (in powers of $1/z$) for the pressure can be directly read⁴ from the Ising LT anti-ferromagnetic polynomials. Unfortunately, the LT anti-ferromagnetic data are scarce and therefore direct methods^{4,5} have been necessary to compute the HA series⁷, presently known only through order 23 for the *sq* lattice, and through the 16th or the 19th orders, respectively for the simple-cubic (*sc*) and the body-centered-cubic (*bcc*) lattices. No such series exist for the lattices with $d > 4$, with which we shall be mainly concerned in this paper.

For the HSLG model one is mainly interested into

a) the leading *nonphysical* singularity²³ of the pressure located at a small negative value of the activity. Its exponent is known to be simply related to that of the universal^{1,24,25} Yang-Lee edge-singularity for spin systems of the same dimension, as well as to the exponents of several other systems²⁶, such as the directed branched polymers, the undirected site or bond animals etc..

b) the parameters of the expected *physical* phase-transition which takes place as the density increases and changes the LD disordered phase into an HD ordered one. In this transition, associated with the nearest singularity of the pressure on the positive activity (or density) axis and accurately checked^{20,27,28} to be Ising-like for the bipartite lattices (to which we shall restrict this study), one of the two equivalent sublattices becomes preferentially occupied at HD, while at LD (or equivalently at LA), the constituents are uniformly distributed all over the lattice sites. We may also remark²⁹ that the transition is “entropy-driven”, because the internal energy vanishes for the allowed configurations of the system and the temperature turns out to be an irrelevant constant, so that the free energy coincides up to a sign with the entropy.

The paper is organized as follows. In Section II, we recall the structure of the LT expansion for a ferromagnetic spin 1/2 Ising model and write down the corresponding LA and LD expansions of the pressure for the HSLG. The analysis of these expansions for lattices of various dimensions, leads to a conjecture on the nature of the nearest singularity in the complex density plane for $d \geq 3$, and is presented in Section III. Simple estimates of the entropy constants for lattices of not too high d are discussed in Section IV. The last Section contains a summary of our results.

The Appendix A0 reviews in some detail our derivation of the LT polynomials of the spin 1/2 Ising model subject to a magnetic field, from the corresponding HT expansion.

In the Appendix A1, we argue that the virial expansion coefficients $v_k(d)$ can be expressed as polynomials in d of degree $\lfloor \frac{k}{2} \rfloor$ and present handy expressions of the LA and the LD expansions of the pressure valid for *hsc* lattices of general dimension.

II. ISING LT EXPANSIONS AND HSLG LA EXPANSIONS

On a finite d -dimensional lattice of N sites (we set the lattice spacing $a = 1$), the spin-1/2 ferromagnetic Ising model in an external magnetic field H , is described by the Hamiltonian^{30,31}

$$\mathcal{H}_N\{\sigma\} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - mH \sum_i \sigma_i \quad (1)$$

where $\sigma_i = -1, +1$ denotes the spin variable at the site i , $J > 0$ is the exchange energy and m (set equal to one in what follows) is the magnetic moment of a spin. The first sum in Eq. (1) extends over all distinct nearest-neighbor pairs of sites, the second sum over all lattice sites. If we set $\beta = 1/k_B T$, $K = J\beta$, with k_B the Boltzmann constant and T the temperature, while $h = H\beta$ denotes the reduced magnetic field, then in the LT and high-field limit, we can write the free energy per site $-\beta\mathcal{F}_{LT}(K, h) = \lim_{N \rightarrow \infty} N^{-1} \ln Z_N(K, h)$ as

$$-\beta\mathcal{F}_{LT}(K, h) = h + \frac{1}{2}qK + \sum_{n=1}^{\infty} L_n^{(1/2)}(u)\mu^n \quad (2)$$

Here $u = \exp[-4K]$, $\mu = \exp[-2h]$, and q is the coordination number of the lattice. The series-expansion coefficients of the free energy in powers of μ , denoted by $L_n^{(1/2)}(u)$, are polynomials in the variable u .

We have recently derived (or, in some cases, extended) the LT expansions of the specific free-energy for the spin- S Ising models, on *hsc* and *bcc* lattices of arbitrary dimension d in presence of a magnetic field. Our additional results were not obtained by extending the direct graphical calculation, but more simply from our high-temperature (HT) expansions¹⁸, by performing on these an appropriate transformation to the LT and high-field variables. In particular, we have derived 13th order LT expansions on the *hsc* lattice of general dimension d , for $S = 1/2$.

As anticipated in the introduction, the knowledge of these expansions yields immediately^{4,5} the coefficients of the LA (LD) expansion for the grand-potential of the HSLG on the same lattices.

For convenience, let us now state a few standard definitions from the statistical mechanics description of the HSLG model. Due to the nearest-neighbor exclusion interaction, the r -th coefficient $g_r(N)$ of the LA expansion of the grand partition-function $\Xi_N(z)$ for a N -site lattice simply counts the allowed configurations of r hard spheres. In the absence of non-hard-core interactions and thus of an energy scale for the system, the statistical mechanics is temperature independent, i.e. the system is “athermal”, and one can simply set $k_B T \equiv 1$. The first three coefficients of the LA expansion of $\Xi_N(z)$ depend on the lattice structure and size N as simply as

$$\Xi_N(z) = \sum_r g_r(N, d) z^r = 1 + Nz + N(N - q - 1)z^2/2! + \dots \quad (3)$$

where $z = \exp(\mu)$ and μ is the chemical potential. It is worth noting that the coefficients $g_r(N, d)$ enumerate the “independent sets” of r vertices in the N -vertex graph induced by the (finite) lattice under study. Thus, in combinatorial language $\Xi_N(z)$ is the “independent-set generating polynomial” of the lattice. Computing these quantities for general graphs has been a much studied problem in combinatorial mathematics³².

In the thermodynamic limit, the coefficients of the LA expansion³³ of the “grand-potential” (or “pressure”) per site

$$\lim_{N \rightarrow \infty} \frac{1}{N} \ln \Xi_N(z) = p(z) = \sum_r c_r(d) z^r = z - \frac{1}{2}(q+1)z^2 + \dots \quad (4)$$

are formally obtained by picking out the coefficients of the terms linear in N in the expansion of $\ln \Xi_N(z)$. In the same limit, the number density of the gas is defined by

$$\rho(z) = \lim_{N \rightarrow \infty} \langle n \rangle / N = z \frac{dp(z)}{dz} = z - (q+1)z^2 + \dots \quad (5)$$

with $\langle n \rangle$ the mean number of hard spheres on the lattice. On the bipartite lattices that we shall consider here, the physical range of the density ρ is $[0, 1/2]$.

The virial expansion of the pressure (LD expansion) is then obtained by using Eq. (5) to express the activity z as function of ρ and substituting it in $p(z)$

$$p(\rho) = \sum_r v_r(d) \rho^r = \rho + \frac{1}{2}(q+1)\rho^2 + \dots \quad (6)$$

The compressibility K_T defined as

$$\rho K_T = \frac{d\rho}{dp} \quad (7)$$

and the specific entropy

$$S = -\rho \ln z + p \quad (8)$$

are also of interest. Note that S vanishes not only as $z \rightarrow 0$, but also as $z \rightarrow \infty$, so that there is no residual entropy at maximum density, since for the bipartite lattices, independently of their structure, the first terms of the HA expansion⁴ for the pressure and the density are $p = \frac{1}{2} \ln z + \frac{1}{2z} + O(\frac{1}{z^2})$ and $\rho(z) = 1/2 - \frac{1}{2z} + O(\frac{1}{z^2})$, respectively.

In the case of the *hsc* lattices, the coefficients $[n, i](d)$ of the various powers of u in the LT polynomials $L_n^{(1/2)}(u)$ can be represented as simple polynomials in d . This property of the LT polynomials reflects the analogous property³⁴ of the HT expansion of the Ising model for this class of lattices. In the Appendix A1, we have discussed why it is so. Correspondingly, we can write simple exact expressions, valid for any d , of each coefficient in the LA and in the LD expansions of the pressure.

These general d expansions for the *hsc* lattices, that we regard as the main result of this paper in spite of their still moderate length, are reported in the Appendix A1. No such simplification is possible for the *hbcc* lattices. In this case, distinct expansions must be written for each value of d and some of them will be tabulated elsewhere.

In the case of the one-dimensional lattice, the free-energy of the Ising model in a field can be computed to all orders yielding exact expressions for the LA expansion of the HSLG model:

$$p(z) = \ln\left(\frac{1 + \sqrt{1 + 4z}}{2}\right) = \sum_{r=1}^{\infty} \frac{(-1)^{r+1}}{r} \binom{2r-1}{r-1} z^r \quad (9)$$

and for the virial expansion

$$p(\rho) = \ln(1 - \rho) - \ln(1 - 2\rho) = \sum_{r=1}^{\infty} \frac{2^r - 1}{r} \rho^r \quad (10)$$

III. SERIES ANALYSES

A. The nonphysical singularity in the complex activity plane

Let us now observe that the LA expansions of the pressure are well suited to estimate numerically the nearest singularity z_d^u in the plane of the complex activity z , which lies on the real negative axis and thus is *nonphysical*, but controls the asymptotic behavior of the coefficients and therefore the convergence radius of the LA expansion. In d dimensions the exponent ϕ_d of this singularity is related^{24,25} to the exponent $\sigma_d = \phi_d - 1$ of the universal Yang-Lee edge-singularity of a ferromagnetic spin system on a lattice of the same dimension d . Using our LA expansions, we can compute the locations and exponents of z_d^u with fair accuracy for all values of d , either with the aid of series-extrapolation prescriptions employing ratios of coefficients^{35,36} or by Padé approximants (PA) or by differential approximants³⁶(DA). In the calculation of the exponent, it is convenient first to locate the singularity as accurately as possible and then use the data so obtained to form biased PAs or DAs. Our estimates for the location z_d^u of the nonphysical singularity and its exponent ϕ_d , generally obtained by first-order DAs using 15th order series on the *hsc* lattices with $d < 5$ or 13th order series otherwise, are shown in the Table I for a few values of d . For the one-dimensional lattice one has exactly $z_1^u = -1/4$ and $\phi_1 = 1/2$. In the case of the *sq* lattice, the high-precision estimates $z_2^u = -0.11933886(5)$ and $\phi_2 = 0.83333(2)$ have been obtained^{8,37-39} by DAs, using the known 92 coefficients of the LA expansion. For $d > 2$, the results cannot reach a comparable accuracy. Completely consistent estimates of z_d^u are always obtained also from the analysis of the LA expansions of the density or of the compressibility.

TABLE I: Estimates of the location of the nearest nonphysical singularities z_d^u of the pressure in the complex activity plane and the corresponding estimates of their exponents ϕ_d for (hyper-)simple-cubic lattices of various dimensions. For $d = 2, 3, 4$, (even when longer expansions are known), we have reported our estimates obtained using only the first 15 coefficients, while for $d > 4$ we have used our 13th order expansions. For comparison, in the second row we have reported early estimates of z_d^u obtained for $d = 2$ and $d = 3$ in Ref.[4,5] from series extending to the 13th and the 11th order respectively. The third and fourth rows list the most accurate estimates of z_d^u and ϕ_d for $d = 2$ from Refs. [8,20,37,38]. The fifth row reports our estimates of ϕ_d from the LA series, the sixth row the estimates of ϕ_d obtained from our high-order LA expansions²⁶ of the hard-dimer density.

	$d = 1$	$d = 2$	$d = 3$	$d = 4$	$d = 5$	$d = 6$	$d = 7$	$d = 8$
z_d^u This work	-0.25	-0.11934(1)	-0.07448(4)	-0.05329(5)	-0.04126(8)	-0.03365(8)	-0.0284(1)	-0.0247(1)
z_d^u Ref.[4,5]		-0.1194(2)	-0.0744(1)					
z_d^u Refs.[8,20,37,38]		-0.11933886(5)						
ϕ_d Refs.[8,20,37,38]		0.83333(2)						
ϕ_d This work	0.5	0.8335(3)	1.08(2)	1.26(5)	1.40(5)	1.45(5)	1.50(5)	1.50(5)
$\sigma_d + 1$ Ref.[26]	0.5	0.8338(5)	1.077(2)	1.258(5)	1.401(9)	1.46(5)	1.495(8)	

In the case of the *hc* lattice, we have estimated $z_{hc}^u = -0.154717(2)$ using the 25th order LA expansion presently available. The corresponding Yang-Lee exponent is $\phi_{hc} = 0.833(2)$.

For the *hpo* lattice, our estimate is $z_{hpo}^u = -0.1498(1)$, with exponent $\phi_{hpo} = 1.08(2)$, based on the known 23rd order LA expansion. From the *diamond* lattice pressure series (17 coefficients), we get $z_{dia}^u = -0.1094(2)$, with exponent $\phi_{dia} = 1.08(2)$.

In the case of the *bcc* lattice, we estimate $z_{bcc}^u = -0.05662(2)$ using the 13th order LA expansion presently available. The exponent estimate is $\phi_{bcc} = 1.08(2)$. Our estimate of z_{bcc}^u has to be compared with the earlier estimate⁵ $z_{bcc}^u = -0.0565(1)$, based on a series shorter by two terms.

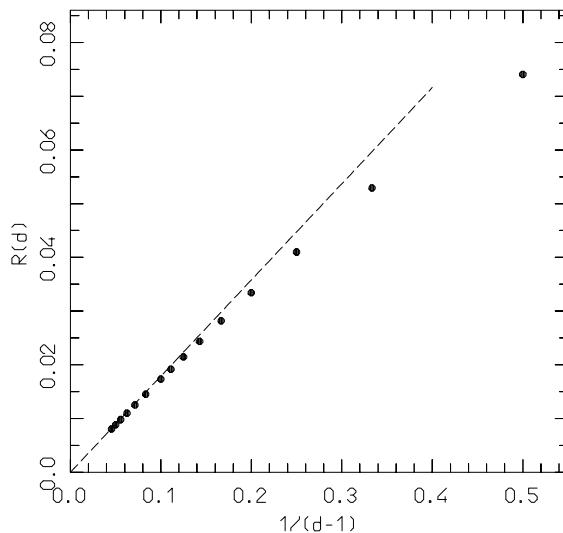


FIG. 1: The estimated radius of the convergence disk of the pressure LA expansion $R(d) = -z_d^u$ for $d = 2, 3, \dots, 23$ is plotted vs $1/(d-1)$ and compared with its expected asymptotic behavior for large d (dashed line).

All the above estimates are in fair agreement with the current most accurate values of the Yang-Lee edge-exponents obtained²⁶ from 24th order hard-dimer density LA expansions, over the same range of values of d , but they are subject to larger uncertainties as they result from an analysis of shorter series.

B. The large d behavior of z_d^u

The structure of the d -dependence of the LA and the LD coefficients in the expansions on the hsc lattices is very suggestive also as far as the large d behaviors are concerned. Observing that on the hsc lattices the LA expansion coefficients $c_n(d)$ are polynomials in d of order $n-1$ and that the convergence radius $|z_d^u|$ of the LA expansion equals the large n limit (assuming that it exists) of the absolute value of the ratios $|c_n(d)/c_{n+1}(d)|$, we can argue that for large d , one has $z_d^u \approx a/d$ with $a = -0.179(5)$. In a slightly better approximation, one can write $z_d^u \approx a/(d-1)$. In the Fig. 1 we have plotted our estimates of $|z_d^u|$ vs $1/(d-1)$ and compared them with their expected asymptotic behavior for large d (dashed line).

C. The physical singularity in the activity

It is not as straightforward to estimate from our LA expansions the critical values of z_d^c associated to the physical phase-transition. Unfortunately, for $d > 2$ our series are not sufficiently long to locate accurately the singularities z_d^c and characterize them as d varies, because $|z_d^c/z_d^u| \gg 1$, as shown by the best current estimates²⁰ obtained by a cluster MC simulation with reduced critical slowdown, and reported in Tab. II for a few values of d . Very accurate estimates of the critical exponents were also achieved in the same study, confirming the Ising-like nature of the transition.

In the case of the one-dimensional lattice, the pressure is analytic for finite positive z (equivalently for $\rho < 1$). For the *sq* lattice, an extremely long LA expansion of $p(z)$ is known, and thus a very accurate estimate of z_2^c could be obtained⁸, in spite of the fact that the physical singularity lies well outside the convergence disk of the expansion.

HA expansions in the variable $1/z$ combined with LA expansions, have also proved helpful^{4,5} in the study of the $d = 2$ and $d = 3$ cases. However HA expansions sufficiently long for this kind of studies are not yet known for $d > 3$.

The existence of a phase transition in the HSLG was first proved in Ref.[40]. More recently⁴¹, the bound $z_d^c = O(d^{-1/4} \ln^{3/4} d)$ has been proved for the *hsc* lattices in d dimensions. Probably this bound is not optimal. The empirical asymptotic formula $z_d^c \approx \frac{e}{2(d-1)} + O(\frac{1}{d^2})$ for large d , agreeing qualitatively with the mean-field approximation, has been devised²⁰ to fit the estimates in Tab. II. In the mean field approximation also ρ_d^c has a similar asymptotic behavior.

Studying term by term the large d behavior of the virial expansion, we can moreover argue that the equation of state should take the form $p = F(\bar{\rho}^2)$, with $\bar{\rho} = \rho\sqrt{d}$ and that the first few terms of the expansion of $F(\bar{\rho}^2)$ in powers of $\bar{\rho}^2$ should be $F(\bar{\rho}^2) = \bar{\rho}^2 - \frac{3}{2}\bar{\rho}^4 - \frac{10}{3}\bar{\rho}^6 - \frac{147}{3}\bar{\rho}^8 - \frac{4536}{5}\bar{\rho}^{10} - \frac{64152}{3}\bar{\rho}^{12} + \dots$. Consistently with the behavior of ρ_d^c , that vanishes in the large d limit, the remark suggests that the equation of state is trivial in this limit.

D. The critical values of the density from the virial expansion

In the case of the one-dimensional lattice, the nearest singularity of the pressure in the complex-density plane occurs at $\rho = 1/2$, just on the upper border of the physical range $0 \leq \rho \leq 1/2$. In dimension $d = 2$, the convergence radius of the LD expansion of the pressure is determined by a complex-conjugate pair of nonphysical singularities in the right-hand half-plane of the complex density, whereas the physical critical value²⁰ of the density lies somewhat farther.

This situation occurs in the *hard-square*, the *hard-triangle* and the *hard-hexagon* model. Unlike the *hc* and *sq* lattice cases, the latter model has been solved exactly^{9,10} and therefore also the nonphysical singularities can be located very accurately.

For the *sq* lattice, we have reanalysed the first 48 coefficients of the LD series looking for the singularities of smallest modulus in the PAs and DAs and have thus obtained the estimate $\rho_2^{nst} = 0.201(5) \pm i0.244(5)$, with modulus $|\rho_2^{nst}| = 0.316(6)$. This result is completely compatible with the early estimate⁴ $\rho_2^{nst} \approx 0.21 \pm i0.26$ from a 12th order series. On the other hand, an accurate recent MC estimate²⁰ of the critical density is $\rho_2^c = 0.367743000(5) > |\rho_2^{nst}|$. It is known^{36,42} that, if the density variable is normalized to the convergence radius $|\rho_2^{nst}|$ of the pressure expansion, the LD expansion coefficients will exhibit asymptotically regular oscillations of constant amplitude and period $L = 2\pi/|\theta|$ inversely proportional to the modulus of the phase θ of the nearest singularity. Using the first 92 coefficients of the long LD expansions reported in Refs.[7,8], we have plotted in Fig. 2 the r th series coefficient in terms of the variable ρ/ρ_2^{nst} vs its order r to exhibit the first few oscillations. Consistently with our estimate of ρ_2^{nst} , an oscillation period tending to $L \approx 7$ is clearly discerned in the plot.

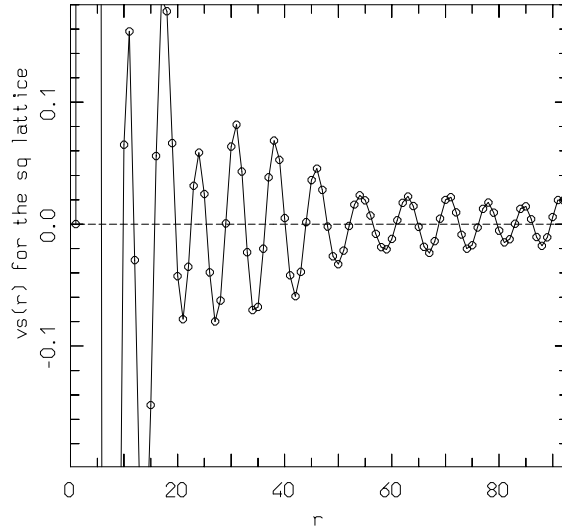


FIG. 2: The r th coefficient $vs(r)$ of the virial expansion (in terms of a density variable normalized with the modulus $|\rho_2^{nst}| = 0.316$ of the nearest singularity in the complex density plane) vs the order r of the coefficient, in the case of the sq lattice. The values of the successive coefficients (open circles) have been interpolated by straight lines to profile more clearly their oscillating behavior. The overall normalization of the curve is arbitrarily chosen for graphical convenience.

Similarly for the sc lattice, we have plotted in Fig. 3 the 15 known LD coefficients vs their order. The plot might either look barely sufficient to guess the onset of a first oscillation, with a period longer than in the $d = 2$ case, or on the contrary to exclude any oscillation. The PA and DA study of the series is similarly inconclusive, suggesting that the nearest singularities are a complex conjugate pair at $\rho_3^{nst} \approx 0.20(6) \pm i0.01(8)$, with modulus $|\rho_3^{nst}| \approx 0.20$. Thus, if oscillations occur in the coefficient plot, their period has to be large, so that they cannot be visible in a plot showing only the first 15 coefficients.

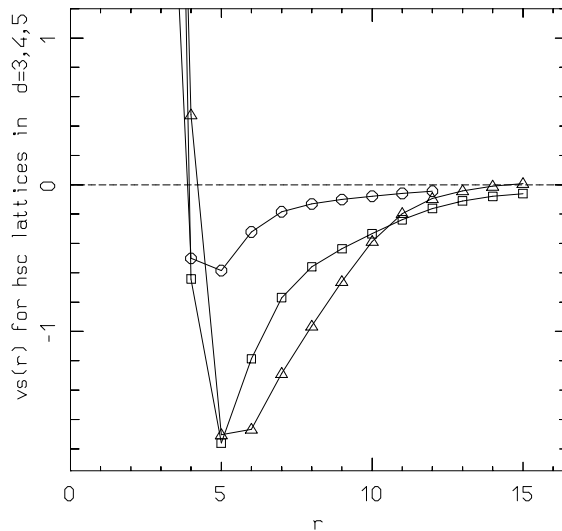


FIG. 3: Same as Fig. 2, for the coefficients of the virial expansions in the cases of the *hsc* lattices in $d = 3$ (open triangles), $d = 4$ (open squares), and $d = 5$ (open circles). For the various curves, the density variables are normalized respectively with $|\rho_3^{nst}| = 0.21$, $|\rho_4^{nst}| = 0.143$ and $|\rho_5^{nst}| = 0.11$, using the estimates of Ref. [20], which are more accurate than ours. The overall normalization of each curve is arbitrarily chosen for graphical convenience.

In the case of dimension $d = 4$, using 15 coefficients, we estimate $\rho_4^{nst} = 0.12(4) \pm i0.01(8)$ and again see no apparent oscillation of the coefficient plot. In the case of dimension $d = 5$, in which 13 coefficients are known, we obtain $\rho_5^{nst} = 0.12(4) \pm i0.02(8)$ and for $d = 6$, we have $\rho_6^{nst} = 0.11(4) \pm i0.001(1)$. For the various dimensions, compatible estimates are also obtained by considering the values of ρ at which the curvature of the pressure vanishes. The corresponding values of z_d are determined from the $\rho = \rho(z)$ curves. No unbiased exponent estimate is possible using our expansions.

Here it is also worth remarking that the virial coefficients $v_r(d)$, whose expressions for the *hsc* lattices are the polynomials in d reported in Appendix A1, are negative for all $d \geq 4$, and $4 \leq r \leq 13$.

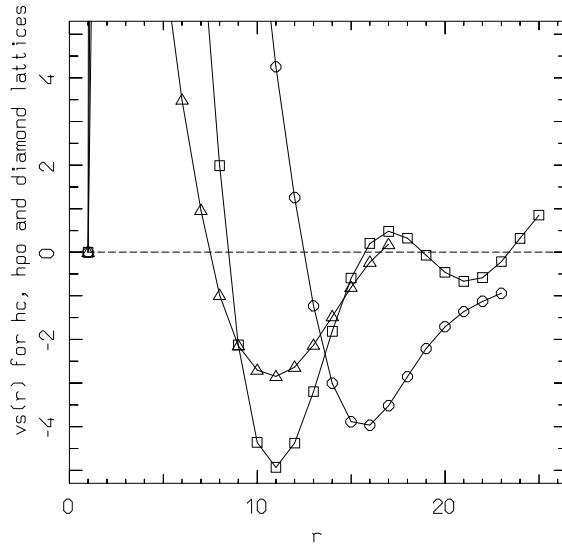


FIG. 4: Same as Fig. 2, for the coefficients of the virial expansions in the cases of the *hc* lattice (open squares), the *hpo* lattice (open circles) and the *diamond* lattice (open triangles). The density variables are normalized respectively with $|\rho_{hc}^{nst}| = 0.38$, $|\rho_{hpo}^{nst}| = 0.36$ and $|\rho_{diam}^{nst}| = 0.31$. The overall normalization of each curve is arbitrarily chosen for graphical convenience.

TABLE II: In the first line, we have reported estimates of the critical activities z_d^c for various d -dimensional *hsc* lattices obtained in Ref.[20,27,38] by a cluster MC simulation. The second line contains the estimates of the critical densities ρ_d^c , obtained by cluster MC methods in Ref.[20,27] for various (hyper)-simple-cubic lattices of dimension d . In the third line, we list our estimates of z_d^{nst} derived from the locations of the nearest singularity ρ_d^{nst} in the density plane. The critical densities are determined by second-order DAs using expansions of order 48, 15, 15, 13, 13 for $d = 2, 3, 4, 5, 6$ respectively and are reported in the fourth line. For $d > 2$, our estimates of the nearest singularity seem to be consistent with those of the critical densities reported in the second line.

	$d = 1$	$d = 2$	$d = 3$	$d = 4$	$d = 5$	$d = 6$
z_d^c Ref.[20,27,38]		3.79625517391234(4)	1.05601(3)	0.58372(1)	0.40259(1)	0.308217(6)
ρ_d^c Ref.[20]		0.367743000(5)	0.210490(3)	0.143334(3)	0.109392(2)	0.088948(2)
z_d^c This work	∞		1.1(3)	0.7(2)	0.5(2)	0.3(1)
ρ_d^{nst} This work	0.5	$0.196(15) \pm i0.243(15)$	$0.21(3) \pm i0.01(8)$	$0.15(3) \pm i0.01(10)$	$0.11(3) \pm i0.02(8)$	$0.09(3) \pm i0.000(1)$

From the results summarized above, we are led to conjecture that, in the case of the *hsc* lattices, either

i) only for $d = 2$, the complex pair of singularities in the density plane coexists with the *farther* singularity on the real axis associated to the physical phase transition, while for $d > 2$ these singularities approach the real axis until they pinch it. For larger values of d , either they coalesce with the physical singularity or replace it. Should this

picture be true, the physical singularity on the positive density axis would become the nearest one for $d \geq 3$ and thus even LD expansions of a moderate length might be of some value in locating it;

or

ii) just like in the $d = 2$ case (and perhaps also for $d = 3$), it is a complex-conjugate pair of singularities in the density plane that determines the convergence radius of the LD expansion also for values of $d \geq 3$. They will approach the real axis asymptotically as d grows and thus the coefficients will show oscillations of increasingly longer, but finite period. Therefore series significantly more extensive than those presented here, would be necessary both to exhibit these oscillations and to locate reliably the critical value of the density ρ_d^{nst} .

To discriminate between the two possibilities, we have compared in Tab.II our series estimates for the nearest singularities in the complex density plane ρ_d^{nst} , from first- and second-order DAs, with the estimates of the critical density ρ_d^c , obtained in Ref.[20]. Of course, for $d > 2$ the accuracy of the computations using our moderately long series is still poor, and unfortunately no simulation study has been attempted to follow the movement of the possible nearest complex singularities for $d > 2$. For $d = 2$, it is well established that $|\rho_2^{nst}| < \rho_2^c$. For $d \geq 3$, we observe that our numerical estimates suggest that $|\rho_d^{nst}| \approx \rho_d^c$, admittedly within large uncertainties. This is consistent with the features of the coefficient plots for the *hsc* lattices in dimensions $d = 3, 4, 5$ shown in Fig. 3. Thus the results of the analysis of our LD series, although not yet allowing sharp conclusions, seem to support the first of the above pictures and encourage us to believe that a reasonable extension of the LD series, might be numerically useful.

We have similarly studied also the LD expansion for the *hc* lattice, the other $2d$ model on a bipartite lattice for which a LA expansion is available, and determined the nearest singularity pair: $\rho_{hc}^{nst} \approx 0.33(2) \pm i0.20(3)$, with modulus $|\rho_{hc}^{nst}| \approx 0.38$. The estimates of the physical critical parameters $z_{hc}^c = 7.92(8)$ and $\rho_{hc}^c = 0.422(10) > \rho_{hc}^{nst}$ of an early study⁴³, are consistent with this result. Thus, as shown in Fig. 4, we expect to see an oscillation of period tending to $L \approx 11$ in the plot of the expansion coefficients (expressed in terms of a density variable normalized to the convergence radius).

On the other hand, in the case of the $3d$ *hpo*, the study of the LD series and the behavior of the LD coefficients, shown in Fig. 4, suggest the location of the nearest singularity in the complex density plane $\rho_{hpo}^{nst} \approx 0.36(1) \pm i0.001(1)$. Consistently the PAs on the compressibility yield $z_{hpo}^c = 5.5(5)$ and $\rho_{hpo}^c = 0.36(1)$. Similarly for the *diamond* lattice, we have $\rho_{dia}^{nst} = 0.31(2) \pm i0.001(1)$ and consistently from PAs on the compressibility we have $z_{diam}^c = 2.8(2)$ and $\rho_{dia}^c = 0.31(2)$. In both cases the physical singularity in the density plane seems to be the nearest one and therefore it can be determined, though still with a significant uncertainty, by the LA and LD expansions. It would be interesting to confirm these estimates by simulations.

In the case of the *bcc* lattice, accurate MC estimates⁴⁴ of the critical activity and of the corresponding critical density are available: the values $z_{bcc}^c = 0.72020(4)$ and $\rho_{bcc}^c = 0.1714(1)$ have been indicated by an MC cluster algorithm. The 13 available LD series-expansion coefficients are too few to give an accurate estimate of the nearest singularities, but, as in the cases of the *sc*, the *hpo* and the *dia* lattices, do not suggest that they are complex.

E. The hard-sphere entropy constants

We can also show that for not too large d , reasonably long LA expansions of the pressure can help to estimate heuristically the constants h_d that control the exponential growth of the number of all possible hard-sphere arrangements over the N sites of a finite d -dimensional *hsc* lattice in the large N limit. These quantities are defined by

$$h_d = S(z)|_{z=1} = \lim_{N \rightarrow \infty} \frac{1}{N} \ln(\Xi_N(z))|_{z=1} = p(1) \quad (11)$$

and are often called *specific-entropy constants of the hard-sphere gas* for the lattice under study. It is easy to show that $p(1)$ is the maximum value of the entropy defined by Eq. (8).

The constants h_d are of interest also in other fields. In information theory, the quantity h_d is called *capacity*⁴⁵ of certain d -dimensional constrained codes used in digital recording applications. As briefly anticipated in Sect. II, the quantity $\Xi_N(1)$, which can be defined for a general graph with N vertices and counts the total number of distinct “independent sets of vertices” i.e. of subsets of pairwise non-adjacent vertices, usually called “vertex-independence-number”⁴⁶ (or Fibonacci number⁴⁷ of the graph) is of interest both in combinatorial mathematics⁴⁸ and in theoretical chemistry. In the latter context it is called Merrifield-Simmons index⁴⁹ and used for a topological characterization of a (large) molecule whose structure is represented by the graph.

We have recently studied⁵⁰ a Grassmann-algebra algorithm that can efficiently compute the “independence polynomial” even for relatively large graphs and in particular for finite lattice graphs. Moreover, extrapolating to infinite lattice the results of this algorithm by the prescriptions of the “finite-lattice-method”⁵¹, we can reproduce at least part of the very long already known LA expansion^{7,8} for the *sq* lattice. Unfortunately our algorithm cannot yet compete with the transfer matrix and thus we cannot extend the existing results.

No closed form expressions are known for the quantities h_d , except for $d = 1$ i.e. $h_1 = \ln((1 + \sqrt{5})/2)$, but for h_2 , h_3 and h_4 rigorous lower and upper bounds have been obtained. In the thoroughly studied^{8,11,38,39} case of the *sq* lattice, a high-precision determination¹¹ of $\exp(h_2) = 1.5030480824753322643220663294755536893857810\dots$ was achieved by extrapolating to infinite lattices variational results from the corner-transfer-matrix method. This value is probably correct¹¹ to 43 decimal places, and is clearly consistent with the rigorous bounds^{45,46,52,53} indicated in Table III. The value of the density at $z = 1$ is $\rho_2(1) = 0.22657081546271468894199226347129902640080\dots$, probably correct¹¹ through the 41 decimal figures reported here. Further improvement of the above estimates by the presently available LA series seems to be out of question. Here we shall be interested only into the higher values of d and use some of the long $d = 2$ expansions mainly to understand the limitations of a simple series resummation method and to support our claim that, at least for not too large d , reasonable estimates of h_d can be obtained even from the moderately long series derived in this paper. To begin with, we show how accurate are the estimates that we obtain for $d = 2$. For example, on the *sq* lattice a naive $[7/7]$ PA which uses only the first 15 coefficients of the LA expansion of $p(z)$, (or better first-order DAs using the same set of coefficients), can reproduce correctly the first four digits of $\exp(h_2) = 1.50305\dots$. Using an increasing number of the many coefficients known for the *sq* lattice, we observe that $p(1)$ and $\rho(1)$, determined in this way, reproduce an increasing number of figures of the above mentioned values and can argue that roughly one more digit of the expected values can be gained for every two additional coefficients used in forming the approximants. Thus it is tempting to test the accuracy of this simple series approach also with the cubic lattices in $3d$ and $4d$, in which only the first 15 coefficients of the LA expansion are known and even to extend this test to higher values of d . From the highest PAs and DAs, we get the estimate $\exp(h_3) = 1.4366(3)$, which is marginally compatible with the known⁵⁴ bounds: $1.4365871627266 \leq \exp(h_3) \leq 1.43781634614$. For the hyper-simple-cubic lattice in $4d$ (again using 15 coefficients), our DA estimate is $\exp(h_4) = 1.394(-5)(20)$. The central value of this estimate lies approximately 2% below the lower end of the range^{22,53} defined by the rigorous inequalities $1.417583 \leq \exp(h_4) \leq \exp(h_3) \leq$ upper bound of $\exp(h_3) = 1.4378\dots$. This upper bound improves marginally the best previous one 1.4447... obtained in Ref.[53]. Even so, the bounds for $d = 4$ remain less tight than for $d < 4$. Finally, using the 13 coefficients derived in dimension $d = 5$, DAs predict $\exp(h_5) = 1.36(-1)(+4)$. Unfortunately, in this case no bound tighter than $\exp(h_5) < \exp(h_4)$ is presently available²², but we can reasonably suppose that our DA results underestimate the correct value by less than 5%. These results indicate that the simplest PAs or DAs can yield relatively accurate analytic continuations of the z -expansion of $p(z)$ well outside their convergence disks (of radius $|z_d^u|$), but also that the precision of this procedure deteriorates rapidly with increasing space dimension d . One reason for this is the shrinking of the convergence radius of the LA expansion (see Table I). Another reason is the decrease of z_d^c as d grows (see Table II). One should also consider that, for $d > 4$, the LA series extend only to 13th order. Since the pressure is expected to be continuous, although non-analytic at z_d^c , one can however hope that longer series might make more accurate estimates possible. Notice for example that, already for $d = 3$ we have $z_3^c \approx 1.056$, while $z_d^c < 1$ for $d \geq 4$. To show how this loss of accuracy as d grows is related to the location of z_d^c , we have plotted in Fig. 5 the quantities $\exp[S(z)]$ vs $z/(1+z)$ for *hsc* lattices of dimension $d = 1, \dots, 6$. They are computed by the PAs of orders $[7/7]$, $[6/6]$ and $[5/5]$ for $d = 1, 2, 3, 4$ and of order $[6/6]$ and $[5/5]$ and $[4/4]$ for $d = 5, 6$, formed with the LA expansions of lengths 15 in the first case and 13 in the second. We have marked by vertical dashed lines the values of $z_d^c/(1+z_d^c)$ to show that, when $d \geq 3$, the convergence of the PAs, that can be judged from the spread of their values for $z \gtrsim z_d^c$, begins to deteriorate before the maxima of the curves are attained, thus making the approximations less reliable. For $d = 2$ and $d = 3$, the known upper and lower bounds of $\exp[S(z)|_{z=1}]$ suggest good approximations of this quantity, indicated in the figure by horizontal continuous lines. For $d = 4$, the available bounds are too loose to be useful in the assessment of the accuracy and we have not indicated them in the figure.

Our estimates of $\exp(h_d)$ for cubical lattices of dimensions $d = 2, 3, \dots, 5$ are summarized in Table III and compared with the upper and lower bounds, whenever available. In the same table we have also reported our estimates of the hard-sphere densities $\rho_d(1)$ in the same approximation. Our central estimates quoted in the tables are obtained as the averages of the highest-order near-diagonal PAs (or DAs) of $p(z)|_{z=1}$, that can be formed from the available LA expansions. To the estimates we have attached uncertainties not smaller than twice the maximum variation among the PA values.

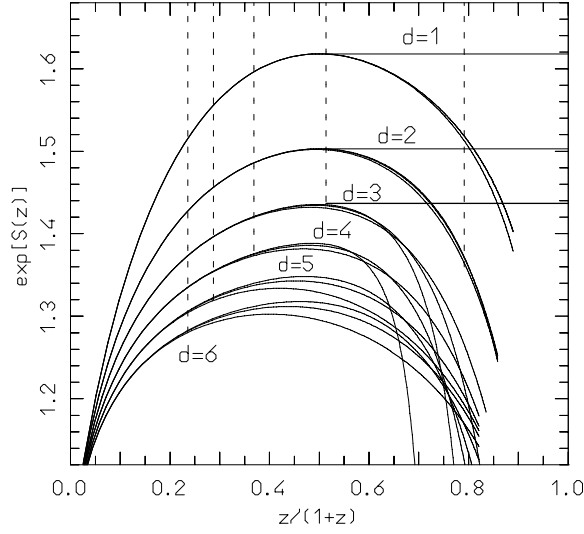


FIG. 5: The exponential of entropy, for the *hsc* lattices, is plotted vs $z/(1+z)$ for $d = 1, 2, 3, \dots, 6$. This quantity is computed by quasi-diagonal PAs formed with 15 series coefficients in dimension $d = 1, 2, 3, 4$ and with 13 coefficients in $d = 5, 6$. The vertical dashed lines indicate the values of $z_d^c/(1+z_d^c)$, for each d . For $d = 1$ the exact result, and for $d = 2, 3$ good approximations for the expected values of $\exp[S(z)]$ at $z = 1$ are indicated by horizontal continuous lines.

F. Entropy constants for other lattices

Transfer-matrix computations¹¹ have yielded high-accuracy estimates also in the case of the *hc* lattice. For the entropy, they give $\exp(h_{hc}) \approx 1.54644070878756141848902270530472278026\dots$, and for the density in $z = 1$, they give $\rho_{hc}(1) \approx 0.2424079763616482188205896378263422541\dots$. Both values are probably correct through the figures reported. Similarly to our previous results, in the case of the *hc* lattice, a $[7/7]$ PA estimate $\exp(h_{hc}) = 1.54642(2)$, reproduces correctly the first four digits of the above value, while the $[12/12]$ PA (that uses all the 25 known coefficients) yields $\exp(h_{hc}) = 1.54644069(2)$ reproducing the first 8 digits. A similar precision is achieved for the corresponding density: the $[7/7]$ PA gives $\rho_{hc}(1) = 0.24240(1)$ and the $[12/12]$ PA gives $\rho_{hc}(1) = 0.2424079(3)$. Moreover, these estimates of $\exp(h_{hc})$ are consistent with the loose inequalities²² $\exp(h_1) > \exp(h_{hc}) > \exp(h_2)$, where $\exp(h_1) = (1 + \sqrt{5})/2 \approx 1.6180\dots$

No earlier estimates are available for the *hpo* lattice. We obtain $\exp(h_{hpo}) = 1.54564(3)$ using a $[7/7]$ PA, while an $[11/11]$ PA yields $\exp(h_{hpo}) = 1.545659(1)$. The corresponding approximations for the density are $\rho_{hpo}(1) = 0.24114(2)$ and $\rho_{hpo}(1) = 0.241153(1)$, respectively. Following Ref.[22], we can expect that $\exp(h_{hpo}) > \exp(h_3)$.

In the case of the *diamond* lattice, we estimate $\exp(h_{dia}) = 1.49526(6)$ and $\rho_{dia}(1) = 0.2188(3)$ and can expect²² that $\exp(h_{dia}) > \exp(h_3)$. We are not aware of tighter bounds for these lattices. Notice that for the *hc*, the *hpo* and

the *diamond* lattices, the critical values of z are $\gg 1$ and thus the accuracy of our entropy estimates is justified. Our PA results for the *hc*, *hpo* and *diamond* lattices are shown in Fig. 6, which differs from Fig. 5 only because $\exp[S]$ is plotted vs ρ instead of $z/(1+z)$.

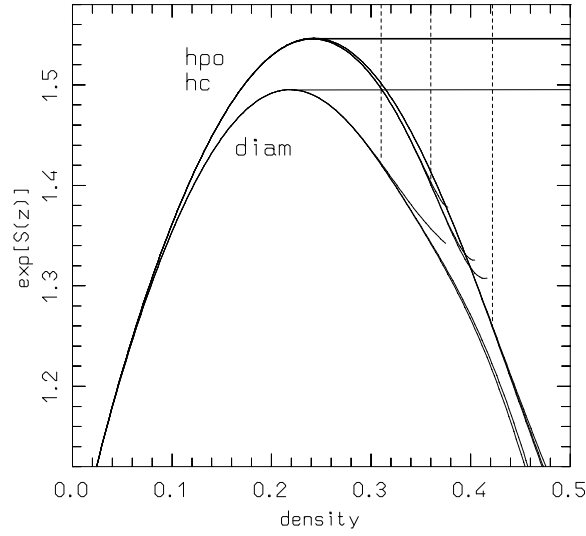


FIG. 6: The exponential of entropy, computed by the highest order available quasi-diagonal PAs, is plotted vs the density ρ for the *hc*, the *hpo* and the *diamond* lattices. We have indicated by vertical dashed lines the values of ρ_c corresponding to the various lattices. Notice that the curves for the *hc* and the *hpo* lattices are indistinguishable on the scale of the figure except in the right hand region.

In the case of the *bcc* lattice, we estimate $\exp(h_{bcc}) = 1.41(2)$ and correspondingly $\rho_{bcc}(1) = 0.21(1)$. The expected inequality²² $\exp(h_{bcc}) < \text{upper bound of } \exp(h_3)$ is satisfied.

TABLE III: DA estimates of the hard-sphere entropy constants $h_d = p(1)$ and the corresponding estimates of the densities $\rho_d(1)$ for (hyper)-simple-cubic lattices of various dimensions. In the second column we have reported tight lower bounds and in the fourth tight upper bounds for h_d on the *hsc* lattice, when available^{45,46,52–54}.

<i>hsc</i>	Lower bound	This work	Upper bound
$\exp(h_2)$	1.503047782	1.50305(2)	1.503058
$\exp(h_3)$	1.4365871627266	1.4366(3)	1.43781634614
$\exp(h_4)$	1.417583	1.394(-5)(20)	1.43781634614
$\exp(h_5)$		1.36(-1)(4)	
$\rho_2(1)$		0.2265(2)	
$\rho_3(1)$		0.202(2)	
$\rho_4(1)$		0.18(2)	
$\rho_5(1)$		0.16(2)	

IV. CONCLUSIONS

Using the results of our recent study of the Ising model HT expansions¹⁸, we have computed through order 13 the LA and LD expansions of the pressure for the HSLG model on the (hyper)-simple-cubic lattices in d dimensions, and written their expressions as polynomials in d through order 13, assuming that the general virial coefficient $v_k(d)$ is a polynomial of degree $\lfloor \frac{k}{2} \rfloor$, as confirmed by our calculations.

With the aid of the current series-extrapolation techniques, we have then analyzed the LA and LD expansions of the pressure for the HSLG model on the (hyper)-simple-cubic lattices, in general dimension d as well as the expansions for the *hc*, the *hpo* and the *diamond* lattices already existing in the literature, but not thoroughly studied. We have thus obtained fairly accurate and nontrivial information, in some cases not previously known, concerning the parameters of the nonphysical singularities and their behaviors as the lattice dimension d grows. As to the more difficult problem of determining the physical singularities by series computations, the presently known expansions for $d > 2$ are still too short to yield estimates that can compete with those from the simulations, but they may help to discuss and justify our conjecture that only in the case of two-dimensional lattices, the nearest singularity in the right-hand plane of the density is a nonphysical complex-conjugate pair. If valid, our conjecture might support the expectation that just somewhat longer expansions can locate reliably the physical singularities also for $d > 2$.

We have also observed that the simplest way to estimate the entropy constants from our series, by PA or DA resummation of the LA series, is very effective for $d = 2$ and $d = 3$, but becomes less accurate for $d > 3$, probably only because the available series are not long enough.

Finally our results suggest that, if the series study of the HSLG model for $d \geq 3$ is considered worth pursuing, a significant extension of the LT series-expansions of the spin 1/2 Ising model in a magnetic field, should be undertaken, because for $d > 2$, the LA and LD expansions can only be derived by following this route.

Acknowledgments

We thank INFN for supporting this research.

V. APPENDIX A0: COMPUTING THE $L_n^{(1/2)}$ FROM THE HT EXPANSIONS

Let $\mathcal{F}(K, H) \equiv \lim_{N \rightarrow \infty} \frac{-1}{N\beta} \ln Z_N(K, H)$ denote the specific free energy for the $S = 1/2$ Ising model subject to a magnetic field H . The corresponding HT series expansion can be written as

$$-\beta \mathcal{F}_{HT}(K, H) = \frac{q}{2} \ln(\cosh(K)) + h + \ln(1 + \mu) + \sum_{i=1}^{\infty} \psi_i(c) t^i \quad (12)$$

Here we have set $h = \beta H$, $c = \tanh(h)$, $\mu = e^{-2h}$ and $t = \tanh(K)$.

The specific free energy is obtained as a HT series, observing that the magnetization $\mathcal{M}(K, h) = -\frac{\partial \mathcal{F}_{HT}}{\partial H} = c + \sum_{i=1}^{\infty} M_i K^i$ can be computed using the linked-cluster method³⁰ in terms of the quantities M_i that are polynomials

in the bare vertices V_i , defined by

$$V_{i+1} = \frac{dV_i}{dh} = ((1 - c^2) \frac{d}{dc})^i c \quad (13)$$

with $V_0 = \ln 2 \cosh(h)$. By integrating the magnetization, one can compute $\mathcal{F}_{HT}(K, H)$ (up to an integration constant depending on K) and thus can determine the quantities $\psi_i(c)$ appearing in Eq. (12), using $\frac{d(-\beta \mathcal{F}_{HT})}{dc} = \frac{\mathcal{M}}{1-c^2}$.

The quantities $\psi_i(c)$ are polynomials in c of degree $2i$, even due to the symmetry $h \rightarrow -h$. The n th order coefficient, in powers of μ , of the LT expansion for high magnetic field results from excitations in which precisely n spins are flipped with respect to the background with all spins up. The LT free energy is given by Eq. (2)

$$-\beta \mathcal{F}_{LT} = K \frac{q}{2} + h + \sum_{k=1}^{\infty} L_k(u) \mu^k \quad (14)$$

where $u = \exp(-4KJ)$. Here and in what follows, for brevity, we shall set $L_k(u) = L_k^{(1/2)}(u)$.

In a domain around infinite magnetic field $\mathcal{F}_{HT}(K, H)$ and $\mathcal{F}_{LT}(K, H)$ are both defined, so they are related by analytic continuation⁵⁵; it is convenient to write the HT variables t and c as

$$t(z) = \frac{1 - \sqrt{1 - z}}{1 + \sqrt{1 - z}} \quad (15)$$

with $z = 1 - u$ and

$$c(\mu) = \frac{1 - \mu}{1 + \mu} \quad (16)$$

Equating the expansions $\mathcal{F}_{LT} = \mathcal{F}_{HT}$ as $K \rightarrow 0$ leads to the identities

$$L_k(1) = (-1)^{k+1}/k \quad (17)$$

while for $h \rightarrow \infty$ one has

$$\frac{q}{2} (\ln(\cosh(K)) - K) + \sum_{i=1}^{\infty} \psi_i(1) t^i = 0 \quad (18)$$

Therefore one gets

$$\sum_{k=1}^{\infty} (L_k(u) - L_k(1)) \mu^k = \sum_{i=1}^{\infty} (\psi_i(c) - \psi_i(1)) t^i \quad (19)$$

Let us denote the coefficient of the power x^r in the Taylor expansion of $f(x)$ at $x = 0$ by $\mathcal{C}_r(f(x)) = \frac{1}{r!} \frac{d^r f}{dx^r} |_{x=0}$, then expanding Eq. (19) about $\mu = 0$

$$L_k(u(z)) = L_k(1) + \sum_{i=1}^{\infty} \mathcal{C}_k(\psi_i(c(\mu))) t(z)^i. \quad (20)$$

The Eq. (20) gives the j -the derivative of L_k in $u = 1$ in terms of $\mathcal{C}_k \psi_1, \dots, \mathcal{C}_k \psi_j$. For instance from $\psi_1 = dc^2$ one obtains the constraint

$$L'_k(1) = dk(-1)^{k+1} \quad (21)$$

$L_k(u)$ is a polynomial of degree $\frac{kq}{2}$ in u , hence the RHS of Eq. (20) has to be a polynomial of the same degree in z . Since $t(z) = O(u)$, the infinite sum is actually a finite sum. The range of the sum is further reduced observing that $L_k(u)$ is a polynomial in u of degree $\frac{kq}{2}$ with the structure

$$L_k(u) = \sum_{r=0}^{\max[N-,]} [k, r] u^{qk/2-r} \quad (22)$$

The notation adopted for the coefficients $[k, r]$ of the polynomial $L_k(u)$ reproduces¹⁵ that commonly used in the literature. In Eq. (22) $r = N_{--}$ is the number of adjacent pairs of flipped spins in the various configurations of k flipped spin described by $L_k(u)$.

Thus $L_k(u)$ contains⁵⁶ only the powers u^r with r ranging from $s_k = \frac{kq}{2} - \max[N_{--}]$ to $\frac{kq}{2}$.

Considering the lattice subgraph whose vertices are the flipped spins and whose edges connect pairs of adjacent flipped spins, it is clear that $\max[N_{--}]$ is the (lattice-dependent) maximum number of links in this class of k -vertex lattice subgraphs.

Thus to compute L_k , it is sufficient to know the HT expansion in a magnetic field through the order $s_k = \frac{kq}{2} - \max[N_{--}]$.

In fact, defining the truncated sum $\mathcal{T}_n(f(x), x) \equiv \sum_{r=0}^n \left(\frac{1}{r!} \frac{d^r f}{dx^r} \Big|_{x=0} \right) x^r$, we get

$$L_k(u) = u^{s_k} \mathcal{T}_{kq/2-s_k} \left((1-z)^{-s_k} \left(\frac{(-1)^{k+1}}{k} + \sum_{i=1}^{kq/2-s_k} t(z)^i \mathcal{C}_k(\psi_i(c(\mu))) \right), z \right) \Big|_{z=1-u} \quad (23)$$

So far, our remarks are true independently of the lattice structure. Let us now restrict to the d -dimensional (hyper)-simple-cubic lattices for which $q = 2d$. For lattices of dimension $d = 0, 1$, the free energy and thus the L_k are known at all orders. We have been able to compute¹⁸ the HT magnetization exactly in terms of c through the order n_d in K , with $n_d = 24$ for $2 \leq d \leq 4$, $n_d = 22$ for $5 \leq d \leq 6$, $n_d = 20$ for $7 \leq d \leq 10$.

For $2 \leq d \leq 4$, we were then able to compute L_k through the following orders: 16th for $d = 2$, 14th for $d = 3$ and 13th for $d = 4$.

Our determination of the L_k for cubic lattices of dimension $d \leq 3$ agrees with the data in the literature⁶. For $d = 4$ we have noticed a single misprint in Ref. [16]: the lowest degree coefficient of L_8 should be $4u^{20}$ instead of $4u^{21}$. For $d > 4$, no data exist in the literature.

In Table IV, we have listed the quantities $kq/2 - \max[N_{--}]$ for $d \leq 4$.

For $d \geq 4$ and $k \leq 16$ it is easy to see that $kd - s_k(d)$ is independent of d . Since a d -dimensional hyper-cube has 2^d vertices, for $k \leq 2^{d-1}$ the graphs with maximal number of links are subgraphs of a $(d-1)$ -hyper-cube, which is a face of the d -hyper-cube. Therefore $kd - s_k(d)$ is the same for the lattices in d and $d-1$ dimensions, if $k \leq 2^{d-1}$. (One can improve this correspondence observing that the graphs with $k \leq 2^d - 2^{d-2}$ vertices and maximal number of links lie on two adjacent 2^{d-1} hyper-cubes, so that $kd - s_k(d)$ is the same for d and $d-1$ if $k \leq 2^d - 2^{d-2}$; however we will not use this remark here). Knowing s_k for $d = 3$ and $k \leq 8$, we can find the corresponding values for $d = 4$ and e.g. can conclude that for $d = 4$ the smallest power of u in the polynomial L_8 is u^{20} .

In $d \geq 5$, for graphs with 16 vertices or less, the vertex configurations with maximal number of links are those on a 4-hypercube forming a face of the d -hyper-cube; therefore $kd - s_k(d)$ is the same as in $d = 4$.

In this way, we have been able to determine the polynomials L_k through the following orders: 13th order in dimension $d = 5, 6$ and 12th in $d = 7, 8, 9, 10$.

TABLE IV: This Table lists the lowest powers $kq/2 - \max[N_{--}]$ of u appearing in L_k for the d -dimensional (hyper)-simple-cubic lattice. The last line gives $\max[N_{--}] = dk - s_k(d)$ for $d \geq 4$, which is the HT order whose knowledge is required to compute L_k from Eq. (23).

d/k	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
2	2	3	4	4	5	5	6	6	6	7	7	7	8	8
3	3	5	7	8	10	11	12	12	14	15	16	16	18	19
4	4	7	10	12	15	17	19	20	23	25	27	28	30	31
$\max[N_{--}]$	0	1	2	4	5	7	9	12	13	15	17	20	22	25

VI. APPENDIX A1: THE ACTIVITY AND VIRIAL EXPANSIONS FOR THE HARD-SPHERE GAS ON THE (HYPER)-SIMPLE-CUBIC LATTICE OF DIMENSION d

In the case of the *hsc* lattices, the coefficients $[k, i](d)$ of the powers of u in the LT-polynomials $L_k^{(1/2)}(u)$ can be expressed as polynomials in the dimension d , of degree $k-1$. Using their values for $d = 0, \dots, 10$, determined as indicated in the previous Appendix, we have been able to write them as polynomials in d through $k = 11$. For $k < 11$, the HT-LT relationship leaves $11 - k$ consistency checks to be satisfied among the coefficients.

The coefficient $[k, 0](d)$ of the highest-order power in u of $L_k(u)$ is the k th coefficient $c_k(d)$ in the LA expansion (Mayer b -series³³) $p = \sum_{r=1}^{\infty} c_r(d)z^r$ of the HSLG model pressure.

Once we have obtained the LA expansion coefficients $c_r(d)$ for $r \leq 11$, the LD expansion coefficients of the pressure (Mayer β -series³³) $p = \sum_{r=1}^{\infty} v_r(d)\rho^r$ are computed through the same order by the standard procedure.

We can observe that for $r \leq 11$, the virial coefficients $v_r(d)$ are polynomials in d of degree $\lfloor \frac{r}{2} \rfloor$ and thus we are led to assume that this property of $v_r(d)$ remains valid for any r . We might argue, more convincingly that this property is a consequence of the fact that the virial expansion uses only one-vertex-irreducible (*star*) Mayer graphs, whose (strong) embedding factors⁵⁵ are themselves polynomials in d of degree at most $\lfloor \frac{r}{2} \rfloor$. A completely analogous argument³⁴ is valid for the HT expansions in general dimension d . Using the coefficients $[k, r](d)$ for $d \leq 6$ and $k \leq 13$, we have then extended our computation of the activity expansion coefficients c_k and hence v_k for $d \leq 6$ and $k \leq 13$, since according to the above remark this is enough to determine the polynomials $v_k(d)$ for $k \leq 13$.

From the virial expansion coefficients $v_k(d)$ with $k \leq 13$, we obtain the activity expansion coefficients $c_k(d)$:

$$c_1(d) = 1$$

$$c_2(d) = -d - 1/2$$

$$c_3(d) = 2d^2 + d + 1/3$$

$$c_4(d) = -16/3d^3 - 3/2d^2 - 5/3d - 1/4$$

$$c_5(d) = 50/3d^4 - 2/3d^3 + 47/6d^2 + 7/6d + 1/5$$

$$c_6(d) = -288/5d^5 + 24d^4 - 118/3d^3 - 4d^2 + 1/10d - 1/6$$

$$c_7(d) = 9604/45d^6 - 882/5d^5 + 1913/9d^4 + 23/6d^3 - 719/45d^2 + 227/30d + 1/7$$

$$c_8(d) = -262144/315d^7 + 47104/45d^6 - 54112/45d^5 + 1079/9d^4 + 11689/90d^3 - 4841/180d^2 - 2743/70d - 1/8$$

$$c_9(d) = 118098/35d^8 - 201204/35d^7 + 6939d^6 - 8272/5d^5 - 21497/40d^4 - 26461/60d^3$$

$$+174025/168d^2 - 37319/140d + 1/9$$

$$c_{10}(d) = -8000000/567d^9 + 640000/21d^8 - 7600000/189d^7 + 139960/9d^6 - 21262/135d^5 + 65629/9d^4$$

$$-12451745/1134d^3 + 294169/252d^2 + 437071/252d - 1/10$$

$$c_{11}(d) = 857435524/14175d^{10} - 449976494/2835d^9 + 219497872/945d^8 - 118160977/945d^7 + 76322413/2700d^6$$

$$-14910479/216d^5 + 1694726807/22680d^4 + 910827493/22680d^3 - 96126973/1400d^2 + 22181029/1260d + 1/11$$

$$c_{12}(d) = -509607936/1925d^{11} + 143327232/175d^{10} - 46669824/35d^9 + 4603392/5d^8 - 62554848/175d^7 + 13448508/25d^6$$

$$-13292172/35d^5 - 51285963/70d^4 + 2776957507/3150d^3 - 1684784/25d^2 - 1891097759/13860d - 1/12$$

$$c_{13}(d) = 551433967396/467775d^{12} - 218615833228/51975d^{11} + 323294840011/42525d^{10} - 18152600453/2835d^9$$

$$+189827943799/56700d^8 - 73090795151/18900d^7 + 1019903740273/680400d^6 + 111272938283/15120d^5 - 4062673959889/680400d^4$$

$$-1208506024709/226800d^3 + 1408813275251/207900d^2 - 22009079311/13860d + 1/13$$

For $d = 3$, two additional coefficients of the LA expansion are known⁶

$$c_{14}(3) = -2544845359479$$

$$c_{15}(3) = 445909846722299/15$$

For $d = 4$, the additional known coefficients are¹⁶

$$c_{14}(4) = -1922838922481311/14$$

$$c_{15}(4) = 11091476544856728/5$$

The virial coefficients $v_r(d)$ are:

$$v_1(d) = 1$$

$$v_2(d) = d + 1/2$$

$$v_3(d) = 2d + 1/3$$

$$v_4(d) = -3/2d^2 + 5d + 1/4$$

$$v_5(d) = -8d^2 + 14d + 1/5$$

$$v_6(d) = -10/3d^3 - 15d^2 + 86/3d + 1/6$$

$$v_7(d) = -40d^3 + 66d^2 - 8d + 1/7$$

$$v_8(d) = -49d^4 + 301/6d^3 + 469/4d^2 - 260/3d + 1/8$$

$$v_9(d) = -784d^4 + 11168/3d^3 - 5716d^2 + 2834d + 1/9$$

$$v_{10}(d) = -4536/5d^5 + 2406d^4 + 5379d^3 - 19314d^2 + 62692/5d + 1/10$$

$$v_{11}(d) = -53984/3d^5 + 417380/3d^4 - 1174120/3d^3 + 1409620/3d^2 - 199446d + 1/11$$

$$v_{12}(d) = -21384d^6 + 348964/3d^5 + 91157/6d^4 - 1087185d^3 + 6211568/3d^2 - 3279380/3d + 1/12$$

$$v_{13}(d) = -495936d^6 + 5617424d^5 - 24986848d^4 + 54097332d^3 - 56281176d^2 + 22049834d + 1/13$$

For $d = 3$ the additional known coefficients of the LD expansion are

$$v_{14}(3) = -425385/2$$

$$v_{15}(3) = 13265929/15$$

For $d = 4$ the additional known coefficients are

$$v_{14}(4) = -1811619255/14$$

$$v_{15}(4) = -2082055915/3$$

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